

Improving the Feshbach–Rubinow approximation

Jean-Marc Richard

Laboratoire de Physique Atomique et Cosmologie
Université Joseph Fourier–CNRS-IN2P3
53, avenue des Martyrs, F-38026 Grenoble cedex, France
email: jean-marc.richard@lpsc.in2p3.fr

PACS: 21.45.+v, 03.65.Ge

February 9, 2008

Abstract

The binding energy of three identical bosons is estimated by coupled differential equations which generalise the Feshbach–Rubinow approximation. This method turns out to be rather efficient, especially in the limit of vanishing binding.

1. Introduction

There is no shortage of methods for solving the quantum-mechanical three-body problem: hyperspherical expansion, Faddeev equations, variational methods with sophisticated search for the free parameters, Monte-Carlo algorithms, etc. Each of them has merits and limitations. For instance, the hyperspherical expansion is a systematic scan of the Hilbert space, and can come in several variants such as “potential harmonics” or “adiabatic”. However, it involves a rather delicate evaluation of the matrix elements of the potential within the basis of harmonics.

In the 50’s, a cleaver approximation, hereafter referred to as FR₁, was proposed by Feshbach and Rubinow [1]. It consists of seeking the bound-state wave function of three identical bosons of mass m as

$$\Psi(x, y, z) = \frac{u(r)}{r^{5/2}} , \quad r = \frac{x + y + z}{2} , \quad (1)$$

where $x = |\mathbf{r}_2 - \mathbf{r}_3|$, $y = |\mathbf{r}_3 - \mathbf{r}_1|$ and $z = |\mathbf{r}_1 - \mathbf{r}_2|$ measure the distances between particles. The S-wave ground state, indeed, depends on three scalar, translation-invariant, variables, which can be chosen as x , y and z . The approximation consists of restricting to a function of their sum. Using astutely the stationnary properties of the Schrödinger equation, Feshbach and Rubinow derived the radial function obeyed by the radial function $u(r)$ and energy E ,

$$-u''(r) + \frac{15}{4r^2}u(r) + 2mV_e(r)u(r) = \frac{14m}{15}u(r)E , \quad (2)$$

where the effective potential results from the projection of the interaction V ,

$$V_e(r) = \int V(x, y, z) d\tau , \quad \int d\tau = \frac{8}{r^5} \int_0^r y dy \int_{r-y}^r (2r - y - z)z dz . \quad (3)$$

This method has been applied to a variety of problems, in particular in nuclear physics [2], and is still used occasionally. However, in the case of baryon spectroscopy [3], the energy provided by FR₁ was found [4] not to be very accurate, as compared, e.g., to the hyperspherical expansion in the approximation of a single partial wave, the so-called hyperscalar approximation (HA).

The best convincing success of FR₁ is perhaps in the domain of loosely-bound systems as encountered for instance in studying Borromean binding [5]. The FR₁

approximation gives a good estimate of the coupling threshold^a g_3 , to be compared to the coupling threshold g_2 of two-body systems.

In Fig. 1, a comparison is made of the three-body binding energy of the simple pairwise exponential potential $V(x, y, z) = g \sum_x v(x)$, with $v(x) = -\exp(-x)$, computed from FR₁ and HA, as a function of the coupling g . The constituent mass is set to $m = 1$. The FR₁ method is clearly much better when the coupling threshold is approached, at $g \sim 1.2$.

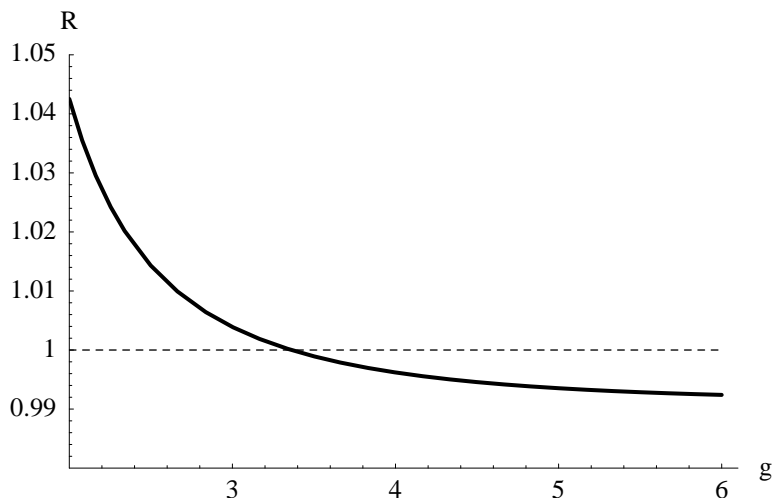


Fig. 1: Ratio of Feshbach–Rubinow to hyperscalar approximations of the three-body energy in a pairwise potential $-g \sum_{i<j} \exp(-r_{ij})$, as a function of the coupling g .

The FR₁ method has been improved by Nogami et al. [2], Rosenthal et al. [6], and in particular adapted to deal with non-identical particles. In spite of its simplicity, the Feshbach–Rubinow method was never extensively used, probably because unlike the HA and other standard methods, it was never presented as the starting point of a converging expansion. We shall suggest below a possible remedy where the three-body wave function is written on a basis of orthogonal polynomials P_i with weight functions $u_n(r)$ that generalise the single $u(r)$ of FR₁ and obey coupled equations.

^a $g \geq g_3$ ensures a three-body bound state in the potential $\sum_{i<j} v(|\mathbf{r}_i - \mathbf{r}_j|)$, where v is attractive or at least, contains attractive parts

The ground-state energy obtained from these coupled equations will be compared to the value given by standard variational methods. For estimating the quality of the wave function, the short-range correlation coefficient $\langle \delta^{(3)}(\mathbf{r}_1 - \mathbf{r}_2) \rangle$ will also be calculated. This quantity enters a number of decay or production rates, and is notoriously hard to compute accurately. Its estimate is sometimes made easier by using identities involving the derivative of the potential and centrifugal terms [4]. We shall restrict ourselves in this paper to a direct reading of the wave function at $\mathbf{r}_1 = \mathbf{r}_2$.

2. Formalism

The FR₁ ansatz is generalised as FR_{*n*}

$$\Psi(x, y, z) = \frac{u_1(r)}{r^{7/2}} P_1(x, y, z) + \frac{u_2(r)}{r^{9/2}} P_2(x, y, z) + \cdots, \quad (4)$$

where P_n is a real and homogeneous polynomial of degree n which is symmetrical. The first one is simply $P_1 = r$, and a truncation there corresponds to the original FR₁ method. Among the polynomials of degree $n = 1$ in x , y and z , only $P_1 \propto x + y + z$, indeed, is symmetric. For $n > 1$, the polynomials $r^{n-1}P_1, \dots, rP_{n-1}$ are already included in the first terms of the expansion (4), hence only a few genuinely new polynomials have to be introduced.^b It is convenient to arrange the P_n to be orthogonal. For $n = 2$, the new polynomial is

$$P_2(x, y, z) = \sqrt{\frac{3}{79}} [72r^2 - 49(x^2 + y^2 + z^2)] , \quad (5)$$

where the coefficient is chosen such that $\int d\tau P_2^2 = r^2 \int d\tau P_1^2$.

If the expansion is truncated there, for testing purposes, the following set of coupled equations can be derived by straightforward calculus:

$$\begin{aligned} \alpha_{11}u_1'' + \frac{\beta_{11}}{r^2}u_1 + \alpha_{12}u_2'' + \frac{\beta_{12}}{r^2}u_2 + \gamma_{12}\frac{u_2'}{r} + V_{11}u_1 + V_{12}u_2 &= \frac{7}{15}\epsilon u_1, \\ \alpha_{22}u_2'' + \frac{\beta_{22}}{r^2}u_2 + \alpha_{21}u_1'' + \frac{\beta_{21}}{r^2}u_1 + \gamma_{21}\frac{u_1'}{r} + V_{21}u_1 + V_{22}u_2 &= \frac{7}{15}\epsilon u_2, \end{aligned} \quad (6)$$

^b For three variables x , y and z , the number p of symmetric polynomials of degree n does not exceed n till $n=5$, and $(p-n)/n$ remains small for $n>5$

with $\epsilon = 2mE$, $\alpha_{11} = -1$, $\alpha_{12} = \alpha_{21} = -2/(5\sqrt{237})$, $\alpha_{22} = -389/395$, $\beta_{11} = 15/4$, $\beta_{12} = -(93/10)\sqrt{3/79}$, $\beta_{21} = -95/(2\sqrt{237})$, $\gamma_{11} = \gamma_{22} = 0$, $\gamma_{12} = -\gamma_{21} = -98/(5\sqrt{237})$. The 2×2 effective potential V_{ij} results from the projections

$$V_{ij} = 2m \int d\tau P_i P_j V(x, y, z) . \quad (7)$$

The coupled equations can be solved by several methods, for instance the discretisation procedure described in [4]. In short, $r \in [0, +\infty[$ is mapped into $x \in [0, 1[$, and if $u_i(r) = v_i(x)$, each v_i is expanded in Fourier series $v_i = \sum_n C_n \sin(n\pi x)$. The coefficients C_n are translated into the values $v_i(x_n)$ of the radial functions at equally-spaced points $x_n = n/(N+1)$, where N is the number of points. The system (6) is reduced to a $2N \times 2N$ matrix equation for the quantities $v_i(x_n)$, and its eigenvalues give a good approximation to the energy levels of (6).

The coefficient of short-range correlation,

$$\delta = \langle \Psi | \delta^{(3)}(\mathbf{x} | \Psi) / \langle \Psi | \Psi \rangle , \quad (8)$$

is given by

$$\delta_1 = \frac{15 \int_0^{+\infty} u^2 r^{-3} dr}{7\pi \int_0^{+\infty} u^2 dr} , \quad \delta_2 = \frac{15 \int_0^{+\infty} r^{-3} [u_1 - 26u_2 \sqrt{3/79}]^2 dr}{7\pi \int_0^{+\infty} [u_1^2 + u_2^2] dr} , \quad (9)$$

for FR_1 and FR_2 , respectively.

3. Results

The method has been first tested on the harmonic oscillator, $v(x) = x^2$ for which the exact solution is $E = 6\sqrt{3/2} \simeq 7.3485$. The FR₁ gives $E_1 = (36/7)\sqrt{15/7} \simeq 7.5284$, and the FR₂ leads to a remarkable improvement, with $E_2 = 7.3537$. Meanwhile, the ratio of short-range correlation δ to the exact value $\delta_{\text{ex}} = (3/2)^{3/4}\pi^{-3/2}$ evolves from $\delta_1/\delta_{\text{ex}} = 1.57$ for FR₁ to $\delta_2/\delta_{\text{ex}} = 0.968$, again a dramatic betterment.

The linear potential $\sum_{i<j} r_{ij}/2 = r$ is diagonal in the basis of polynomials P_i , but is not exactly solvable because the kinetic energy is not diagonal. The results are $E_1 \simeq 3.906$ for FR₁ and $E_2 \simeq 3.8635$ for FR₂, to be compared with $E_{L=0} \simeq 3.8647$ and $E_{L\leq 4} \simeq 3.8633$ in the hyperspherical expansion with one and two partial waves, respectively [4]. The correlation coefficient is estimated to be $\delta_1 = 0.08488$ for FR₁ and $\delta_2 = 0.05592$ for FR₂. For comparison, $\delta \simeq 0.05689$ is obtained from four coupled hyperspherical waves [4], and $\delta \simeq 0.05702$ from 176 correlated Gaussians, a method to be presented shortly.

As for the short-range potentials, let us take again the example of the exponential potential $v(x) = -g \exp(-x)$ already considered in the introduction. Figure 2 displays the ratio of FR₂ to FR₁ ground-state energy as a function of the coupling g : the improvement saturates at about 2% at large coupling and becomes more interesting in the domain of very weak binding.

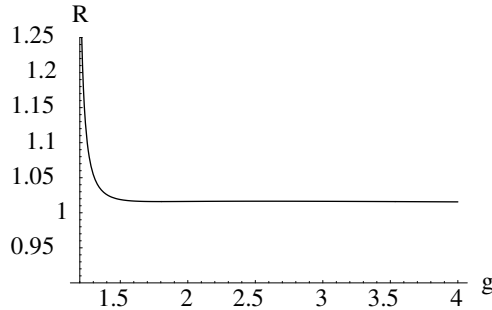


Fig. 2: Ratio of FR₂ to FR₁ approximations of the three-body energy in a pairwise potential $-g \sum_{i<j} \exp(-r_{ij})$, as a function of the coupling g .

In Fig. 3, our results are compared with these of one the fashionable methods on the market. It consists of expanding the wave function on a basis of correlated Gaussians

$$\Psi(x, y, z) = \sum_i C_i \left\{ \exp \left[-(a_i \mathbf{v}^2 + 2b_i \mathbf{v} \cdot \mathbf{w} + c_i \mathbf{w}^2)/2 \right] + \dots \right\} , \quad (10)$$

written in terms of the Jacobi variables

$$\mathbf{v} = \mathbf{r}_2 - \mathbf{r}_1, \quad \mathbf{w} = \frac{2\mathbf{r}_3 - \mathbf{r}_1 - \mathbf{r}_2}{\sqrt{3}}, \quad (11)$$

where the dots are meant for Gaussians deduced by permutation of the particles. Varga and Suzuki [7] have pushed the method of stochastic search of the parameters to a high degree of efficiency, and obtained very accurate estimates of binding energies in a variety of domains. We shall use here the strategy of Hiyama et al. [8]: Gaussians with diagonal quadratic forms, i.e., $a_i \mathbf{v}^2 + c_i \mathbf{w}^2$, are first introduced, and if $a_i \neq c_i$, they are supplemented by the terms deduced by permutation, which includes an angular dependence through $\mathbf{v} \cdot \mathbf{w}$ and carry the same weight factor C_i to ensure Bose symmetry. The range parameters a_i and c_i are chosen to be any member of a geometric series $\{a, ar, ar^2, \dots, ar^{N-1}\}$. This means that, however large is the number of terms, only two non-linear parameters, a and r , are to be optimised. Note that $N = 2$ range parameters correspond to $N' = 8$ Gaussians, $N = 3$ to $N' = 21$, $N = 4$ to $N' = 40$, i.e., a fairly large number of terms.

The plots in Fig. 3 indicate that the FR_2 value is better than this variational estimate with $N = 2$, especially at vanishing binding, comparable to $N = 3$, and is defeated shortly by $N = 4$. This means that FR_2 is roughly equivalent to an expansion involving 40 correlated Gaussians, at least for this particular potential.

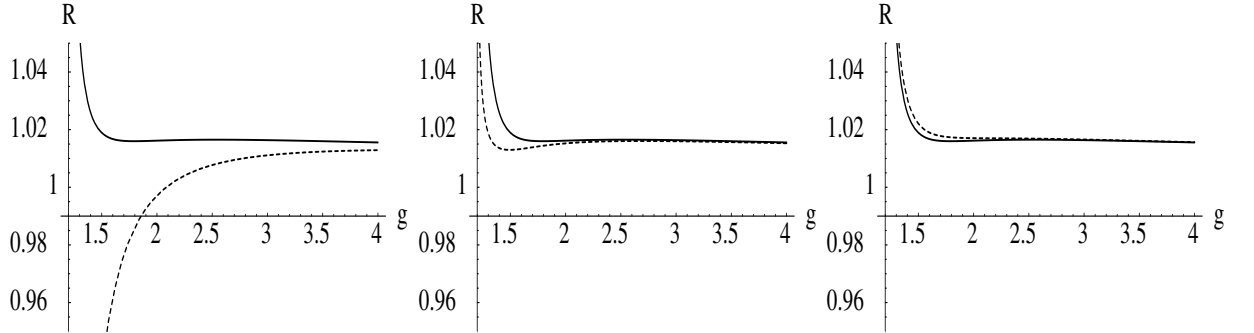


Fig. 3: Comparison of the energy in the exponential potential, as a function of the coupling g , for the FR_2 approximation (solid line), and the Gaussian expansion (dashed line) with $N = 2$ range parameters (left), $N = 3$ (centre) and $N = 4$ (right), corresponding to $N' = 8, 20, 40$ terms. For clarity, the energies are shown by their ratio to the FR_1 approximation.

For further checking, a basis of correlated exponential functions has also been used, namely

$$\psi(x, y, z) = \sum_i C_i [\exp(-a_i x - b_i y - c_i z) + \dots] , \quad (12)$$

where the dots mean terms deduced by circular permutations of $\{a_i, b_i, c_i\}$. Wave functions of this type have been used in pioneering works on few-charge systems and in recent high-precision calculations of atomic systems [9]. The strategy of Ref. [8] can also be applied, to avoid numerical instabilities in the minimisation process, by restricting all range parameters a_i, b_i, \dots to belong to a single geometric series. Note that with suitable constraints on these range parameters, this method can mimic the FR1 method ($a_i = b_i = c_i \ \forall i$) or its generalisation [6] by Rosenthal and Haracz (RH), ($\{a_i, b_i, c_i\} \propto \{a_1, b_1, c_1\} \ \forall i > 1$), $r^{5/2}u(r)$ being described as a sum of exponentials. This provides a check of the numerical solution of the radial FR1 equation or its RH analogue.

In Ref. [6], indeed, Rosenthal et al. proposed to replace the symmetric ansatz $F(r) = u(r)/r^{5/2}$, $2r = x + y + z$ of FR1 by

$$\Psi(x, y, z) = F(\eta_1 x + \eta_2 y + \eta_3 z) + \dots , \quad (13)$$

where the dots correspond to permutation of x , y and z to restore the symmetry of the wave function. This method results in an integro-differential equation for F , whose solution is further optimised by varying η_2 and η_3 empirically (a normalisation $\eta_1 = 1/2$ can be adopted).

In Table 1, a comparison is made of the values obtained for the ground-state energy and correlation coefficient in the exponential potential at coupling $g = 1.4$ and of the critical coupling g_3 at which three-body binding occurs. FR₁ and FR₂ are compared to RH, as well as to the Gaussian expansion GN with up to N different values of the range parameters, and its analogue EN with exponentials.

At least with this potential, and for this domain of coupling close to the stability threshold, the generalisation of the Feshbach–Rubinow approximation with two coupled differential equations, FR₂, appears as more efficient than the single integro-differential equation RH. The ground-state energy, short-range correlation and coupling threshold approaches the exact value to about 1% accuracy for the simple exponential potential.

Table 1. Ground-state energy E_3 and correlation coefficient δ for an exponential potential with coupling $g = 1.4$, and critical coupling g_3 for three-body binding, with FR_1 , FR_2 and RH methods and variational calculations using correlated Gaussian (G) or exponential (E) basis functions with varying number of allowed range parameters.

	$G2$	$G4$	$G8$	$E2$	$E4$	$E5$	FR_1	RH	FR_2
$-E_3$	0.03055	0.03575	0.03586	0.03466	0.03583	0.03586	0.03468	0.03475	0.03542
δ	0.00840	0.00972	0.01000	0.01251	0.01005	0.01002	0.01212	0.01224	0.01091
g_3	1.2194	1.1613	1.1563	1.2158	1.1587	1.1560	1.1751	1.1649	1.1644

4. Outlook

In this paper, the Feshbach–Rubinow method is generalised by expanding the ground-state wave-function of three identical bosons on orthogonal polynomials of the interparticle distances. The coefficients of these polynomials are functions of the sum of distances and obey coupled equations which can be derived by calculus and solved numerically. The results obtained with two equations provide a dramatic improvement in the case of confining potentials where the single-equation version of this method was known to be inaccurate. For the short-range potentials, the results are also significantly better, and become really excellent in the limit of loose binding,

Further investigations would be necessary to check the convergence when the number of equations is increased, and for excited states. The accuracy of the method should also be probed for potentials with hard core, which often occur in applications. The case of particles with different masses or interaction properties also deserves further work. The binding energy and wave function of the positronium ion and other two-electron atoms, which were the subject of interesting developments of the Feshbach–Rubinow method, will be studied in a forthcoming paper within the formalism of coupled equations.

Acknowledgments: I would like to thank Elian Masnada for stimulating discussions that led to this study, and Muhammad Asghar for very useful comments on the manuscript.

References

- [1] H. Feshbach and S.I. Rubinow, Phys. Rev. **98** (1955) 188.
- [2] Leila Abou-Hadid and K. Higgins, Proc. Phys. Soc. **79** (1962) 34; D. Maroun and M. McMillan, Nucl. Phys. A **159** (1970) 661; R.K. Bhaduri and Y. Nogami, Phys. Rev. A **13** (1976) 1986; S.G. Lie, Y. Nogami and M.A. Preston, Phys. Rev. A **18** (1978) 787; Zhongzhou Ren, J. Phys. G: Nucl. Part. Phys. **20** (1994) 1185; Phys. Rev. C **49** (1994) 1281.
- [3] R.K. Bhaduri, L.E. Cohler and Y. Nogami, Phys. Rev. Lett. **44** (1980) 1369.
- [4] J.-M. Richard, Phys. Rep. **212** (1992) 1.
- [5] C.M. Rosenthal and R.D. Haracz, J. Chem. Phys. **76**, 1040 (1982); Phys. Rev. A **25** (1982) 1846.
- [6] J. Goy, J.-M. Richard, and S. Fleck, Phys. Rev. A **52** (1995) 3511.
- [7] Y. Suzuki, K. Varga, *Stochastic variational approach to quantum mechanical few-body problems*, Springer-Verlag, (Berlin, Heidelberg) 1998.
- [8] E. Hiyama, Y. Kino and M. Kamimura, Prog. Part. Nucl. Phys. **51** (2003) 223.
- [9] See, e.g., H.A. Bethe and E.E. Sapleter, *Quantum Mechanics of one- and two-electron atoms* (Plenum, New-York) 1977; A.M. Frolov, Phys. Rev. A **69** (2004) 022505; E.A.G. Armour et al., Phys. Rep. **413** (2005) 1; and refs. therein.